



ERRORF - A Code to Calculate Covariance of Self-shielding Factor and Its Temperature Gradient

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ERRORF - A Code to Calculate Covariance of Self-shielding Factor and Its Temperature Gradient

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A computer code, ERRORF, was developed for calculation of covariance of self-shielding factor and its temperature gradient. This code is based on several modules. With this code, covariance of self-shielding factor and its temperature gradient can be calculated from evaluated nuclear data library in the ENDF format. The installation and calculation methods are explained with sample input and output.

Keywords: Self-shielding Factor, Temperature Gradient, Covariance, Resolved Resonance Parameter, Sensitivity Coefficient, ERRORF

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ERRORF - 自己遮蔽因子及びその温度勾配の共分散計算コード

日本原子力研究開発機構
次世代原子力システム研究開発部門
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自己遮蔽因子とその温度勾配の共分散を計算するためのコード ERRORF を開発した。このコードは幾つかのモジュールから構成されている。このコードにより、ENDF 形式に格納された評価済み核データライブラリに基づいた自己遮蔽因子とその温度勾配の共分散を計算することができる。本レポートでは、導入方法と計算方法を入出力例とともに示す。

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1 Introduction

Doppler reactivity has been recognized as one of the most important safety parameters among the self regulation characteristics of reactors, and high accuracy in the prediction of the reactivity has been vigorously sought in reactor design. In standard sensitivity analyses of nuclear characteristics, the relative sensitivity of a nuclear characteristic R to the infinite dilution cross section $\hat{\sigma}_\infty$, $S_{R,\sigma} = (\hat{\sigma}_\infty/R)(\partial R/\partial \hat{\sigma}_\infty)$ has been used. The sensitivity analysis code SAGEP [1] has used this relative sensitivity coefficient for improvement in adjusted reactor constants with fixed self-shielding factors. This formalism, however, is not applicable to temperature-related nuclear characteristics such as Doppler reactivity because such characteristics depend on the self-shielding factor as well as the infinite dilution cross section. Regarding the temperature gradient of the self-shielding factor as a “pseudo cross section”, the relative sensitivity of the temperature-related nuclear characteristic R to the temperature gradient of the self-shielding factor α , $S_{R,\alpha} = (\alpha/R)(\partial R/\partial \alpha)$, can be introduced. If the temperature gradient α is defined by the logarithmic derivative of the self-shielding factor with respect to temperature, the coefficients $S_{R,\alpha}$ can be obtained from the sensitivity coefficients of effective neutron multiplication factor k_{eff} to the infinite dilution cross section $S_{k_{\text{eff}},\sigma}$ [2].

The ERRORF code has been developed to calculate covariances of the self-shielding factor and its temperature gradient from the resonance parameter covariance matrix and the sensitivity of the self-shielding factor and its temperature gradient to the resonance parameters.

In this manual, we briefly summarize the formalism used in this code. Then installation and input/output of the ERRORF code system are explained with an example of input and output files.

The main reference of the ERRORF code [3] shows more detailed background and theoretical description of this work with an evaluation for uranium-238 capture reaction. In addition, evaluation for uranium-235, uranium-238, plutonium-239 and plutonium-240 are reported elsewhere [4].

2 Formalism

We define the g -th group self-shielding factor $f_{i,c}^g(T, \sigma_b)$ and its temperature gradient $\alpha_{i,c}^g(T, \sigma_b)$ as follows,

$$f_{i,c}^g(T, \sigma_b) = \frac{\hat{\sigma}_{i,c}^g(T, \sigma_b)}{\hat{\sigma}_{i,c,\infty}^g}, \quad (1)$$

$$\alpha_{i,c}^g(T, \sigma_b) = \frac{1}{f_{i,c}^g(T, \sigma_b)} \frac{\partial f_{i,c}^g(T, \sigma_b)}{\partial T}, \quad (2)$$

where

$$\hat{\sigma}_{i,c,\infty}^g = \hat{\sigma}_{i,c}^g(T_{\text{ref}}, \sigma_b = \infty) \quad (3)$$

is the infinite dilution cross section calculated at a reference temperature T_{ref} ^{*}. Two suffixes i and c refer nuclide and reaction channel considered. Hereafter we omit temperature and background cross section dependence as well as these suffixes.

Error propagation from resonance parameter to self-shielding factor and its temperature gradient is written as

$$\theta_{gg'} \frac{\delta f^g}{f^g} \frac{\delta f^{g'}}{f^{g'}} = \sum_{i,j} \frac{x_i}{f^g} \frac{\partial f^g}{\partial x_i} \frac{x_j}{f^{g'}} \frac{\partial f^{g'}}{\partial x_j} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} = \sum_{i,j} s_i^g s_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \quad (4)$$

$$\tau_{gg'} \frac{\delta \alpha^g}{\alpha^g} \frac{\delta \alpha^{g'}}{\alpha^{g'}} = \sum_{i,j} \frac{x_i}{\alpha^g} \frac{\partial \alpha^g}{\partial x_i} \frac{x_j}{\alpha^{g'}} \frac{\partial \alpha^{g'}}{\partial x_j} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} = \sum_{i,j} S_i^g S_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \quad (5)$$

where

- $\theta_{gg'}$: Correlation matrix of self-shielding factor $\{f^g\}$
- $\tau_{gg'}$: Correlation matrix of temperature gradient $\{\alpha^g\}$
- x_i : Resonance parameter $\boldsymbol{x}=\{x_i\}=(E_{r,1}, \Gamma_{n,1}, \Gamma_{\gamma,1}, \dots)$
- ρ_{ij} : Correlation matrix of resonance parameter \boldsymbol{x}
- δx_i : Absolute standard deviation of resonance parameter x_i
- s_i^g : Relative sensitivity coefficient of self-shielding factor f^g to resonance parameter x_i
- S_i^g : Relative sensitivity coefficient of temperature gradient α^g to resonance parameter x_i .

The relative sensitivity coefficients s_i^g and S_i^g are defined as

$$s_i^g(\boldsymbol{x}, T) = \frac{x_i}{f^g(\boldsymbol{x}, T)} \frac{\partial f^g(\boldsymbol{x}, T)}{\partial x_i}, \quad (6)$$

$$S_i^g(\boldsymbol{x}, T) = \frac{x_i}{\alpha^g(\boldsymbol{x}, T)} \frac{\partial \alpha^g(\boldsymbol{x}, T)}{\partial x_i}. \quad (7)$$

The summations in Eqs. (4) and (5) are taken over all resolved resonance parameters. By equating g to g' in Eqs. (4) and (5), we obtain the relative variances of the self-shielding factor and its temperature gradient in the g -th group,

$$\left(\frac{\delta f^g}{f^g} \right)_{\text{tot}}^2 = \sum_{i,j} s_i^g s_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}, \quad (8)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g} \right)_{\text{tot}}^2 = \sum_{i,j} S_i^g S_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j}. \quad (9)$$

These are simplified if we ignore contribution of correlation and consider only contribution of variance,

$$\left(\frac{\delta f^g}{f^g} \right)_{\text{var}}^2 = \sum_i (s_i^g)^2 \left(\frac{\delta x_i}{x_i} \right)^2, \quad (10)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g} \right)_{\text{var}}^2 = \sum_i (S_i^g)^2 \left(\frac{\delta x_i}{x_i} \right)^2. \quad (11)$$

* $T_{\text{ref}}=600$ K is used in the reference [3].

From Eqs. (4) and (5), the correlation matrices $\theta_{gg'}$ and $\tau_{gg'}$ can be expressed as

$$\theta_{gg'} = \left(\sum_{i,j} s_i^g s_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) \Big/ \left(\frac{\delta f^g}{f^g} \frac{\delta f^{g'}}{f^{g'}} \right), \quad (12)$$

$$\tau_{gg'} = \left(\sum_{i,j} S_i^g S_j^{g'} \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) \Big/ \left(\frac{\delta \alpha^g}{\alpha^g} \frac{\delta \alpha^{g'}}{\alpha^{g'}} \right). \quad (13)$$

Sometimes resolved resonance parameters are divided into some intervals which introduce a submatrix structure to the covariance matrix of resonance parameters,

$$\mathbf{V} = \begin{pmatrix} \mathbf{V}^1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^2 & \mathbf{0} \\ & & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{V}^n \end{pmatrix}, \quad (14)$$

where \mathbf{V} is the resonance parameter covariance matrix and \mathbf{V}^l is the resonance parameter covariance submatrix in the l -th energy interval.

The right hand sides of Eqs. (8) and (9) are accordingly decomposed as

$$\left(\frac{\delta f^g}{f^g} \right)_{\text{tot}}^2 = \sum_{l \in L_g} \left(\sum_{i,j \in M_l} s_i^g s_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) \quad (15)$$

$$\left(\frac{\delta \alpha^g}{\alpha^g} \right)_{\text{tot}}^2 = \sum_{l \in L_g} \left(\sum_{i,j \in M_l} S_i^g S_j^g \rho_{ij} \frac{\delta x_i}{x_i} \frac{\delta x_j}{x_j} \right) \quad (16)$$

where L_g means the set of energy intervals overlapping with the g -th group, and M_l means the set of all resonance parameters of the levels in the l -th interval. Note that s_i^g and S_i^g are zero if $i \in M_l$ and $l \notin L_g$ because we assume that the cross section in an energy interval in L_g is not sensitive to the change in the i -th resonance parameter which is not in the energy interval L_g .

3 Modules

A brief description of modules in ERRORF is given in this section.

- (1) **READCOV**: To read nuclear data file in the ENDF-6 format [5], and output resonance parameter covariance matrix.
- (2) **CHECKCOV**: To prepare list of resonance levels to which covariances are evaluated.
- (3) **NJOYINPUTMAKER**: To prepare the input file of njoy.
- (4) **REPCHANGE**: To read nuclear data file in the ENDF-6 format, and to change the i -th resonance parameter x_i in \boldsymbol{x} to obtain a modified parameter set \boldsymbol{x}_i , where the i -th parameter is changed from x_i to $(1 + \epsilon)x_i$.

- (5) **NJOY:** To construct cross section $\sigma(\mathbf{x}_i, E, T)$ from the modified resonance parameter set \mathbf{x}_i , and to calculate the self-shielding factor $f^g(\mathbf{x}_i, T, \sigma_b)$ from the effective cross sections $\hat{\sigma}(\mathbf{x}_i, T, \sigma_b)$ and infinite dilution cross sections $\hat{\sigma}(\mathbf{x}_i, T_{\text{ref}}, \sigma_b = \infty)$ according to Eq. (2).
- (6) **FTOALPHA:** To obtain the temperature gradient $\alpha^g(\mathbf{x}_i, T)$ and sensitivity coefficients $s_i^g(\mathbf{x}, T)$ and $S_i^g(\mathbf{x}, T)$ from the partial derivatives of $f^g(\mathbf{x}_i, T)$ with respect to the resonance parameter and temperature. The partial derivative with respect to resonance parameters was performed by the forward difference formula, while the partial derivative with respect to temperatures is obtained by the three-point central difference formula for numerical accuracy. Namely, $\alpha^g(\mathbf{x}_i, T)$, $s_i^g(\mathbf{x}, T)$ and $S_i^g(\mathbf{x}, T)$ are obtained as

$$\alpha^g(\mathbf{x}_i, T) = \frac{1}{f^g(\mathbf{x}_i, T)} \frac{f^g(\mathbf{x}_i, T + \Delta T, \sigma_b) - f^g(\mathbf{x}_i, T - \Delta T, \sigma_b)}{2\Delta T}, \quad (17)$$

$$s_i^g(\mathbf{x}, T) = \frac{x_i}{f^g(\mathbf{x}, T)} \frac{f^g(\mathbf{x}_i, T, \sigma_b) - f^g(\mathbf{x}, T, \sigma_b)}{\Delta x_i}, \quad (18)$$

$$S_i^g(\mathbf{x}, T) = \frac{1}{\alpha^g(\mathbf{x}, T)} \frac{s_i^g(\mathbf{x}, T + \Delta T, \sigma_b) - s_i^g(\mathbf{x}, T - \Delta T, \sigma_b)}{2\Delta T}. \quad (19)$$

- (7) **WRITESEN:** To output list of sensitivity coefficients.
- (8) **FATABLE:** To output list of self-shielding factor and its temperature gradient at temperature T .
- (9) **ERRPROP:** To calculate standard deviations $\delta f^g/f^g$ and $\delta \alpha^g/\alpha^g$, and correlation $\theta_{gg'}$ and $\tau_{gg'}$ according to the error propagation Eqs. (4) and (5).

4 Installation

4.1 Requirements

The following softwares are required:

- Fortran compiler (to compile some modules during installation)
- Perl system (to execute some perl scripts during calculation)
- NJOY system (to obtain self-shielding factors during calculation)

The ERRORF code has been tested in a Linux machine (DualCore Intel Xenon Processor 5110 1.6GHz and SuSE Linux Ver.7.3) with g77 fortran and njoy99.161. The description in this manual is for UNIX systems.

4.2 Installation

In order to install the ERRORF code, please gunzip the distributed file “errorf.tar.gz”.

```
% gunzip errorf.tar.gz
% tar xvf errorf.tar
```

Then the following file structure should be generated.

```
errorf---+--code----+--checkcov.pl
|           +-fatable.pl
|           +-ftoalpha.f
|           +-ftoalpha (must be prepared from ftoalpha.f by users)
|           +-ftoalpha.pl
|           +-errprop.f
|           +-errprop (must be prepared from errprop.f by users)
|           +-njoyinputmaker.f
|           +-njoyinputmaker
|               (must be prepared from njoyinputmaker.f by users)
|           +-readcov.f
|           +-readcov (must be prepared from readcov.f by users)
|           +-repchange.pl
|           +-writesen.pl
|           +-Makefile
|
+-jendl---+-j33-u238.txt (for test run)
|           +- (add your library file)
|
+-njoy----+-xnjoy (must be prepared by users)
|
+-readme---+--readme.pdf
|           +-readme.txt (a short manual)
|           +-readme_readcov.txt
|
+-test----+--errorf.inp
|           +-errorf.sh
|           +-group.inp
|           +-prenjoy.inp
```

```

|      +-out----+sample.product_1.dat
|              +-sample.product_2.dat
|              +-sample.product_3.dat
|
+- (add your working directory)

```

4.3 Configuration

After generation of this file structure, the following three set up works must be done:

- (1) Prepare four executables “ftoalpha”, “njoyinputmake”, “errprop” and “readcov” from “ftoalpha.f”, “njoyinputmaker.f”, “errprop.f” and “readcov.f” as follows:

```
% make
```

- (2) Find executable file of the NJOY system [7], and put it under the directory “njoy” with the file name “xnjoy”. The NJOY executable file is not included in the ERRORF system distribution.
- (3) Set paths in *.sh and *.pl file according to your environment. Default paths in these files are /bin/csh and /usr/bin/perl for csh and Perl, respectively.

5 Execution with Sample Input

After installation, users can learn how to use the ERRORF code by using the set of sample input files in the directory “test”, where calculation of covariance of self-shielding factor and its temperature gradient for uranium-238 neutron capture based on JENDL-3.3 [6] is considered as an example.

5.1 Get resonance level scheme

5.1.1 Prepare getlevel.inp

Prepare an input file “getlevel.inp”. This input file specifies orbital angular momentum considered in the calculation.

Input specifications:

- * card 1
endf_input (name of input file in endf format)
- * card 2

```

imode (always 0)
* card 3
lvalue (orbital angular momentum, 9 for all  $l$ )
(end of file)

```

Example 1:

Below is an example “getlevel.inp”, where s-wave is considered.

```

./jendl/j33-u238.txt
0
0

```

5.1.2 Execute ERRORF to get level scheme

```
% errorf.sh < getlevel.inp
```

Then you should get “list_lev.txt” as follows.

Example 2:

Below is an example of “list_lev.txt”.

#	Seq.	L	Eres (eV)	Gam(n) (eV)	Gam(g) (eV)
	1	0	-4.405250E+03	1.085500E+02	2.300000E-02
	2	0	-4.133000E+02	7.072100E-02	2.300000E-02
	3	0	-3.933000E+02	6.898900E-02	2.300000E-02
	4	0	-3.733000E+02	6.721200E-02	2.300000E-02
	5	0	-3.533000E+02	6.538700E-02	2.300000E-02
					
	556	0	1.040760E+04	2.205000E-01	2.300000E-02
	557	0	1.041300E+04	4.520000E-02	2.300000E-02
	558	0	1.042640E+04	4.610000E-02	2.300000E-02
	559	0	1.046480E+04	9.600000E-02	2.300000E-02
	560	0	1.049290E+04	8.335000E-01	2.300000E-02
	561	0	1.448490E+04	1.805100E+02	2.732600E-02

You find level index in the first column (“Seq.”) of this file. This level index is used in “prenjoy.inp” which will be described later.

5.2 Input files for NJOY calculation

Prepare 2 input files, “prenjoy.inp” and “group.inp”.

5.2.1 prenjoy.inp

This input file gives some basic parameters of the NJOY calculation. Note that number of background cross sections (nsigz) is fixed to 9.

Input specifications:

- * card 1
iwt (weighting function, see the NJOY manual)
- * card 2
nsigz (number of background cross sections, always 9)
- * card 3
sigz (set of background cross sections)
- * card 4
nmt (number of reaction channel to be calculated)
- * card 5
mtnum (set of reaction channel in mt scheme, see table 1) (end of file)

Example 3:

Below is an example of “prenjoy.inp”, with which self-shielding factor and its temperature gradient are calculated for 2 reaction channels (nmt=2), i.e. fission reaction (mt=18) and capture reaction (mt=102), at 9 background cross sections (nsigz=9), i.e. $\sigma_b = 10^{10}, 10^6, 10^5, 10^4, 10^3, 10^2, 37, 1, 10^{-1}$ barn with weighting function of “Maxwell distribution + (1/E) + fission neutron distribution” (iwt=6).

```

6 / iwt
9 / nsigz
1e10 1e6 1e5 1e4 1e3 1e2 37. 1. 0.1 / sigz
2 / nmt
18 102 / mtnum(1)

```

5.2.2 group.inp

Prepare an input file “group.inp”. This gives group structure in output files.

Input specifications:

* card 1a
 ngroup (number of groups)
 * card 1b
 eh (ngroup+1 group breaks in eV)
 (end of file)

Example 4:

Below is an example of “group.inp”, where the JAERI Fast Set-3 (JFS-3) 70 group structure is given.

```
70
1.0000000E-05 3.2241900E-01 4.1399400E-01 5.3157900E-01 6.8256000E-01
8.7642500E-01 1.1253500E+00 1.4449800E+00 1.8553900E+00 2.3823700E+00
3.0590200E+00 3.9278600E+00 5.0434800E+00 6.4759500E+00 8.3152900E+00
1.0677000E+01 1.3709600E+01 1.7603500E+01 2.2603300E+01 2.9023200E+01
3.7266500E+01 4.7851200E+01 6.1442100E+01 7.8893200E+01 1.0130100E+02
1.3007300E+02 1.6701700E+02 2.1445400E+02 2.7536500E+02 3.5357500E+02
4.5399900E+02 5.8294700E+02 7.4851800E+02 9.6111700E+02 1.2341000E+03
1.5846100E+03 2.0346800E+03 2.6125900E+03 3.3546300E+03 4.3074300E+03
5.5308400E+03 7.1017400E+03 9.1188200E+03 1.1708800E+04 1.5034400E+04
1.9304500E+04 2.4787500E+04 3.1827800E+04 4.0867700E+04 5.2475200E+04
6.7379500E+04 8.6517000E+04 1.1109000E+05 1.4264200E+05 1.8315600E+05
2.3517700E+05 3.0197400E+05 3.8774200E+05 4.9787100E+05 6.3927900E+05
8.2085000E+05 1.0539900E+06 1.3533500E+06 1.7377400E+06 2.2313000E+06
2.8650500E+06 3.6787900E+06 4.7236700E+06 6.0653100E+06 7.7880100E+06
1.0000000E+07
```

5.3 Main calculation

5.3.1 Make output directory

Make directory “out” under your working directory, where NJOY output files are saved.

5.3.2 errorf.inp

Prepare an input file “errorf.inp”. This input file gives basic parameters of the ERRORF calculation.

Input specifications:

- * card 1
endf_input (name of input file in endf format)
- * card 2
imode (always 1)
- * card 3
lvalue (orbital angular momentum, 9 for all l , must be same as getlev.inp)
- * card 4
lev_min (minimum index of level taken from list_lev.txt)
- * card 5
lev_max (maximum index of level taken from list_lev.txt)
- * card 6
phq_min (minimum index of physical quantity to which sensitivity is considered, see Table 1).
- * card 7
phq_max (maximum index of physical quantity to which sensitivity is considered, see Table 1).
- * card 8
temp (temperature in calculation of temperature gradient, T in Eqs. (17) – (19) in Kelvin.)
- * card 9
dtemp (step of temperature in calculation of temperature gradient, ΔT in Eqs. (17) – (19) in Kelvin.)
- * card 10
tempref (reference temperature in calculation of temperature gradient, T_{ref} in Eq. (3) in Kelvin.)
- * card 11
factor (modification factor to resonance parameter in calculation of sensitivity, ϵ)
- * card 12
freac (index of reaction channel to be calculated, see Table 1)
- * card 13
isig0 (index of background cross section to be calculated listed in the card 3 of prenjoy.inp)

(end of file)

Example 5:

Below is an example of “errorf.inp”, where sensitivity of capture width of the 22-th level to self-shielding factor and its temperature gradient for capture reaction at temperature $T=800$ K is calculated with a temperature step $\Delta T=200$ K, reference temperature $T_{\text{ref}}=0$ K, modification factor 1.05, and the 7-th background cross section in prenjoy.inp.

```
./jendl/j33-u238.txt
```

Table 1: Definition of physical quantity index and reaction index

index	physical quantity	index	reaction channel
1	E_r (resonance energy)	1	total
2	Γ_n (neutron width)	2	elastic
3	Γ_g (capture width)	18	fission
4	Γ_{fa} (first partial fission width)	102	capture
5	Γ_{fb} (second partial fission width)		

1
0
22
22
3
3
800
200
0
1.05
102
7

5.3.3 Run ERRORF

```
% errorf.sh < errorf.inp >& errorf.log &
```

Execution time for the sample input (1 physical quantity and 1 resonance level) is about 7 min on a DualCore Intel Xenon Processor 5110 (1.6 GHz). Usually total calculation time is proportional to number of quantities times number of levels.

5.4 Output

5.4.1 Main output files

If the system is properly installed and the test calculation is done, we get 3 main outputs after the ERRORF calculation

- product_1.dat Variances for f-factor and its temperature gradient (See Eqs. (8) – (11)).
 product_2.dat Contribution of energy intervals to f-factor's temperature gradient (See Eq. (16)).
 product_3.dat Correlation matrix for f-factor and its temperature gradient (See Eqs. (12) and (13)).

Another example of outputs from these three files can be seen in Table 2 to 5 in the reference [3].

Example 6:

Below is an example of “product_1.dat” obtained in the test run.

Grp	Ehigh	f	df/f	df/f	a	da/a	da/a
			tot	var	*1e-4	tot	var
(ev)			(%)	(%)	(/deg)	(%)	(%)
49	6.1442E+01	1.0061	0.0005	0.0005	0.0306	0.0000	0.0000
50	4.7851E+01	0.6398	0.0000	0.0000	0.5384	0.0000	0.0000
51	3.7267E+01	0.0308	0.0000	0.0000	0.4830	0.0000	0.0000
52	2.9023E+01	0.9747	0.0000	0.0000	0.0662	0.0000	0.0000
53	2.2603E+01	0.0447	0.0000	0.0000	1.1949	0.0000	0.0000
54	1.7604E+01	1.0051	0.0005	0.0005	0.0346	1.3943	1.3943
55	1.3710E+01	0.9987	0.0020	0.0020	0.0263	1.9403	1.9403
56	1.0677E+01	0.9920	0.0078	0.0078	0.0979	0.4338	0.4338
57	8.3153E+00	0.0480	0.8597	0.8597	1.2504	1.6886	1.6886
58	6.4760E+00	0.8285	0.5156	0.5156	1.0289	1.8684	1.8684
59	5.0435E+00	1.0019	0.0005	0.0005	0.0422	0.0005	0.0005
60	3.9279E+00	1.0014	0.0005	0.0005	0.0220	0.5505	0.5505
61	3.0590E+00	1.0010	0.0005	0.0005	0.0155	1.5629	1.5629
62	2.3824E+00	1.0007	0.0005	0.0005	0.0110	1.1013	1.1013
63	1.8554E+00	1.0006	0.0000	0.0000	0.0112	1.0773	1.0773
64	1.4450E+00	1.0007	0.0000	0.0000	0.0127	0.9506	0.9506
65	1.1254E+00	1.0005	0.0000	0.0000	0.0095	0.0000	0.0000
66	8.7643E-01	1.0007	0.0000	0.0000	0.0130	0.0000	0.0000
67	6.8256E-01	1.0008	0.0000	0.0000	0.0155	0.0000	0.0000
68	5.3158E-01	1.0003	0.0000	0.0000	0.0067	0.0000	0.0000
69	4.1399E-01	1.0002	0.0000	0.0000	0.0052	0.0000	0.0000
70	3.2242E-01	0.9912	0.0082	0.0082	0.0005	2.4315	2.4315

Example 7:

Below is an example of “product_2.dat” obtained in the test run.

Grp	Eh	da/a	rsx1	rsx2	rsx3	rsx9	rsx10
		(ev)	%	%	%	%	%
49	6.1E+1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
50	4.8E+1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
51	3.7E+1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
52	2.9E+1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
53	2.3E+1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
54	1.8E+1	1.3943	1.3943	0.0000	0.0000	0.0000	0.0000
55	1.4E+1	1.9403	1.9403	0.0000	0.0000	0.0000	0.0000
56	1.1E+1	0.4338	0.4338	0.0000	0.0000	0.0000	0.0000
57	8.3E+0	1.6886	1.6886	0.0000	0.0000	0.0000	0.0000
58	6.5E+0	1.8684	1.8684	0.0000	0.0000	0.0000	0.0000

59	5.0E+0	0.0005	0.0005	0.0000	0.0000	0.0000	0.0000
60	3.9E+0	0.5505	0.5505	0.0000	0.0000	0.0000	0.0000
61	3.1E+0	1.5629	1.5629	0.0000	0.0000	0.0000	0.0000
62	2.4E+0	1.1013	1.1013	0.0000	0.0000	0.0000	0.0000
63	1.9E+0	1.0773	1.0773	0.0000	0.0000	0.0000	0.0000
64	1.4E+0	0.9506	0.9506	0.0000	0.0000	0.0000	0.0000
65	1.1E+0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
66	8.8E-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
67	6.8E-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
68	5.3E-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
69	4.1E-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
70	3.2E-1	2.4315	2.4315	0.0000	0.0000	0.0000	0.0000

Example 8:

Below is an example of “product_3.dat” obtained in the test run.

correlation matrix for alpha value

.....	54	55	56	57	58	59	60	61	62	63	64	70
49	0	0	0	0	0	0	0	0	0	0	0
50	0	0	0	0	0	0	0	0	0	0	0
51	0	0	0	0	0	0	0	0	0	0	0
52	0	0	0	0	0	0	0	0	0	0	0
53	0	0	0	0	0	0	0	0	0	0	0
54	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
55	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
56	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
57	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
58	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
59	-99	-99	-99	-99	-99	100	100	100	100	-99	-99 100
60	-99	-99	-99	-99	-99	100	100	100	100	-99	-99 100
61	-99	-99	-99	-99	-99	100	100	100	100	-99	-99 100
62	-99	-99	-99	-99	-99	100	100	100	100	-99	-99 100
63	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
64	100	100	100	100	100	-99	-99	-99	-99	100	100 -99
65	0	0	0	0	0	0	0	0	0	0	0 0
66	0	0	0	0	0	0	0	0	0	0	0 0
67	0	0	0	0	0	0	0	0	0	0	0 0
68	0	0	0	0	0	0	0	0	0	0	0 0
69	0	0	0	0	0	0	0	0	0	0	0 0
70	-99	-99	-99	-99	-99	100	100	100	100	-99	-99 100

correlation matrix for f-factor

49	54	55	56	57	58	59	60	61	62	63	70
49	100	-99	100	-99	-99	100	100	-99	-99	-99	0 100
50	0	0	0	0	0	0	0	0	0	0	0 0
51	0	0	0	0	0	0	0	0	0	0	0 0
52	0	0	0	0	0	0	0	0	0	0	0 0
53	0	0	0	0	0	0	0	0	0	0	0 0
54	-99	100	-99	100	100	-99	-99	100	100	100	0 -99

55	100	-99	100	-99	-99	100	100	-99	-99	-99	0	100
56	-99	100	-99	100	100	-99	-99	100	100	100	0	-99
57	-99	100	-99	100	100	-99	-99	100	100	100	0	-99
58	100	-99	100	-99	-99	100	100	-99	-99	-99	0	100
59	100	-99	100	-99	-99	100	100	-99	-99	-99	0	100
60	-99	100	-99	100	100	-99	-99	100	100	100	0	-99
61	-99	100	-99	100	100	-99	-99	100	100	100	0	-99
62	-99	100	-99	100	100	-99	-99	100	100	100	0	-99
63	0	0	0	0	0	0	0	0	0	0	0	0
64	0	0	0	0	0	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0	0	0	0	0	0
66	0	0	0	0	0	0	0	0	0	0	0	0
67	0	0	0	0	0	0	0	0	0	0	0	0
68	0	0	0	0	0	0	0	0	0	0	0	0
69	0	0	0	0	0	0	0	0	0	0	0	0
70	100	-99	100	-99	-99	100	100	-99	-99	-99	0	100

5.4.2 Other output files

In addition to main output files, we get 4 types of output under working directory “out”:

ffactor_mnnnn	f-factor table
ftoalpha_mnnnn	sensitivity coefficient table
endf_mnnnn	modified endf file
gendf_mnnnn	modified gendif file
output_mnnnn	njoy output

m denotes an index of physical quantity modified ($1 \leq m \leq 5$, defined in Section 5.2). *n* denotes an index of resonance level modified (defined in “list_lev.txt” explained in Section 5.1.2).

“ffactor_mnnnn” has 6 columns:

Igrp	Group index
Ehigh	Upper boundary energy (eV)
ffact (0)	$f^g(\mathbf{x}_i, T_{\text{ref}})$
ffact (1)	$f^g(\mathbf{x}_i, T - \Delta T)$
ffact (2)	$f^g(\mathbf{x}_i, T)$
ffact (3)	$f^g(\mathbf{x}_i, T + \Delta T)$

“ftoalpha_mnnnn” has 8 columns (See also Eqs. (18), (17) and (19)):

Igrp	Group index
Ehigh	Upper boundary energy (eV)
alph3	$\alpha^g(\mathbf{x}_i, T)$
sfpr3 (1)	$s_i^g(\mathbf{x}, T - \Delta T)$
sfpr3 (2)	$s_i^g(\mathbf{x}, T)$
sfpr3 (3)	$s_i^g(\mathbf{x}, T + \Delta T)$
dsft3	$[s_i^g(\mathbf{x}, T + \Delta T) - s_i^g(\mathbf{x}, T - \Delta T)]/2T$
sapr3	$S_i^g(\mathbf{x}, T)$

5.5 Analysis for various reactionchannels/background cross sections

In the ERRORF code, one ERRORF run provides self-shielding factors and related quantities for a set of reaction channels and background cross sectoions (σ_b) defined in prenjoy.inp, and these are stored under the working directory "out".

There is a limitation that the final output file of the ERRORF code is for one reaction channel and one background cross section defined in the 12th and 13th card of "errorf.inp". Hence, the ERRORF code has an option to utilize self-shielding factors and ralated quantities stored in the working directory. With this option, you can obtain results for other reaction cross sections / background cross sections without NJOY calculations as long as you keep the NJOY output files under directory "out".

Example 9:

Below is an example of for a calculation without NJOY run. This looks similar to Example 5, but NJOY calculation is skipped (the 2nd card is 2). In this case, you obtain results at the 6th sig0 (background cross section) in the NJOY input is used (the 13th card is 6) for the fission reaction (the 12th card is 18).

```
./jendl/j33-u238.txt
2
0
22
22
3
3
800
200
0
```

1.05

18

6

Then rerun errorf with “recalc.inp”

```
% errorf.sh < recalc.inp >& recalc.log&
```

6 Conclusion

The ERRORF code was developed to evaluate covariance of self-shielding factor and its temperature gradient. The current version covers resonance parameters expressed by the Reich-Moore formalism and other expression is not supported yet. In addition, unresolved resonance is also outside of the scope of the current version because of limitation of covariance expression in the current ENDF format. Extension of the current version to these data expressions must be done in future as needs arise.

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国際単位系 (SI)

表1. SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表2. 基本単位を用いて表されるSI組立単位の例

組立量	SI 基本単位	
	名称	記号
面積	平方メートル	m^2
立体角	立体度メートル	m^3
速度	速度メートル毎秒	m/s
加速度	度メートル毎秒毎秒	m/s^2
波数	メートル毎秒	m^{-1}
密度(質量密度)	密度キログラム毎立方メートル	kg/m^3
質量体積(比体積)	体積立法メートル毎キログラム	m^3/kg
電流密度	度アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
(物質量)濃度	モル毎立方メートル	mol/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率	(数の)1	1

表3. 固有の名称とその独自の記号で表されるSI組立単位

組立量	SI 組立単位		
	名称	記号	他のSI単位による表し方
平面角	ラジアン ^(a)	rad	$m \cdot m^{-1} \cdot s^{-1}$ ^(b)
立体角	ステラジアン ^(a)	sr ^(c)	$m^2 \cdot m^{-2} = 1$ ^(b)
周波数	ヘルツ	Hz	s^{-1}
圧力	ニュートン	N	$N \cdot m^2$
応力	パスカル	Pa	$N \cdot m^{-1}$
エネルギー、仕事、熱量	ジュール	J	$N \cdot m$
工率、放熱	ワット	W	J/s
電荷、電気量	クーロン	C	$kg \cdot m^2 \cdot A \cdot s^{-3}$
電位差(電圧)、起電力	ボルト	V	W/A
静電容量	フアード	F	C/V
電気抵抗	オーム	Ω	V/A
コンダクタンス	ジemens	S	A/V
磁束密度	テスラ	T	$V \cdot s$
イシダクタンス	ヘンリイ	H	Wb/m^2
セルシウス温度	セルシウス度 ^(d)	°C	$kg \cdot s^{-2} \cdot A^{-1}$
光束度	ルーメン	lm	$cd \cdot sr^{(c)}$
(放射性核種の)放射能吸収線量、質量エネルギー一分率、カーマ	ベクレル	Bq	lm/m^2
線量当量、周辺線量当量、方向性線量当量、個人線量当量、組織線量当量	グレイ	Gy	J/kg
			$m^2 \cdot s^{-2}$
			J/kg
			$m^2 \cdot s^{-2}$

(a)ラジアン及びステラジアンの使用は、同じ次元であっても異なる性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときのいくつかの用例は表4に示されている。

(b)実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号“1”は明示されない。

(c)測光学では、ステラジアンの名称と記号srを単位の表し方の中にそのまま維持している。

(d)この単位は、例としてミリセルシウス度m°CのようにSI接頭語を伴って用いても良い。

表4. 単位の中に固有の名称とその独自の記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa · s	$m^{-1} \cdot kg \cdot s^{-1}$
力のモーメント	ニュートンメートル	N · m	$m^2 \cdot kg \cdot s^{-2}$
表面張力	ニュートンメートル	N/m	$kg \cdot s^{-2}$
角速度	ラジアン毎秒	rad/s	$m \cdot m^{-1} \cdot s^{-1}$
角加速度	ラジアン毎平方秒	rad/s ²	$m \cdot m^{-1} \cdot s^{-2}$
熱流密度、放射照度	ワット每平方メートル	W/m ²	$kg \cdot s^{-3}$
熱容量、エントロピー	ジュール毎ケルビン	J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$
質量熱容量(比熱容量)	ジュール每キログラム	J/(kg · K)	$m^2 \cdot s^{-2} \cdot K^{-1}$
質量エントロピー	毎ケルビン		
質量エネルギー(比エネルギー)	ジュール每キログラム	J/kg	$m^2 \cdot s^{-2} \cdot K^{-1}$
熱伝導率	ワット每メートル毎ケルビン	W/(m · K)	$m \cdot kg \cdot s^{-3} \cdot K^{-1}$
体積エネルギー	ジュール每立方メートル	J/m ³	$m^{-1} \cdot kg \cdot s^{-2}$
電界の強さ	ボルト每メートル	V/m	$m \cdot kg \cdot s^{-3} \cdot A^{-1}$
体積電荷	クーロン每立方メートル	C/m ³	$m^{-3} \cdot s \cdot A$
電気変位	クーロン每平方メートル	C/m ²	$m^{-2} \cdot s \cdot A$
誘電率	ファラード每メートル	F/m	$m^{-3} \cdot kg^{-1} \cdot s^4 \cdot A^2$
透磁率	ヘンリー每メートル	H/m	$m \cdot kg \cdot s^{-2} \cdot A^{-2}$
モルエネルギー	ジュール每モル	J/mol	$m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$
モルエントロピー	ジュール每モル每ケルビン	J/(mol · K)	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1} \cdot mol^{-1}$
モル熱容量	クーロン每キログラム	C/kg	$kg^{-1} \cdot s \cdot A$
照射線量(X線及びγ線)	クーロン每キログラム	C/kg	$kg^{-1} \cdot s \cdot A$
吸収線量率	グレイ每秒	Gy/s	$m^2 \cdot s^{-3}$
放射強度	ワット每平方メートル	W/m ²	$m^4 \cdot m^{-2} \cdot kg \cdot s^{-3} = m^2 \cdot kg \cdot s^{-3}$
放射輝度	ワット每平方メートル每ステラジアン	W/(m ² · sr)	$m^2 \cdot m^{-2} \cdot kg \cdot s^{-3}$

表5. SI 接頭語

乗数	接頭語	記号	乗数	接頭語	記号
10^{-24}	ヨタ	Y	10^{-1}	デシ	d
10^{-21}	ゼタ	Z	10^{-2}	センチ	c
10^{-18}	エクサ	E	10^{-3}	ミリ	m
10^{-15}	ペタ	P	10^{-6}	マイクロ	μ
10^{-12}	テラ	T	10^{-9}	ナノ	n
10^9	ギガ	G	10^{-12}	ピコ	p
10^6	メガ	M	10^{-15}	フェムト	f
10^3	キロ	k	10^{-18}	アト	a
10^2	ヘクト	h	10^{-21}	ゼット	z
10^1	デカ	da	10^{-24}	ヨクト	y

表6. 国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h=60 min=3600 s
日	d	1 d=24 h=86400 s
度	°	$1^\circ=(\pi/180) \text{ rad}$
分	'	$1'=(1/60)^\circ=(\pi/10800) \text{ rad}$
秒	"	$1''=(1/60)'=(\pi/648000) \text{ rad}$
リットル	L	$1L=dm^3=10^{-3}m^3$
トン	t	$1t=10^3 \text{ kg}$
ネーベル	Np	$1Np=1$
ベル	B	$1B=(1/2) \ln 10(Np)$

表7. 国際単位系と併用されこれに属さないSI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位であらわされる数値
電子ボルト	eV	$1eV=1.60217733(49) \times 10^{-19} J$
統一原子質量単位	u	$1u=1.6605402(10) \times 10^{-27} \text{ kg}$
天文単位	ua	$1ua=1.49597870691(30) \times 10^{11} \text{ m}$

表8. 国際単位系に属さないが国際単位系と併用されるその他の単位

名称	記号	SI 単位であらわされる数値
海里	里	1海里=1852m
ノット	ト	1ノット=1海里每時=(1852/3600)m/s
アード	a	$1a=1 \text{ dam}^2=10^2 \text{ m}^2$
ヘルツ	ha	$1ha=1 \text{ hm}^2=10^4 \text{ m}^2$
バル	bar	$1 \text{ bar}=0.1 \text{ MPa}=100 \text{ hPa}=10^5 \text{ Pa}$
オングストローム	Å	$1 \text{ Å}=0.1 \text{ nm}=10^{-10} \text{ m}$
バーン	b	$1 \text{ b}=100 \text{ fm}^2=10^{-28} \text{ m}^2$

表9. 固有の名称を含むCGS組立単位

名称	記号	SI 単位であらわされる数値
エルグ	erg	$1 \text{ erg}=10^{-7} \text{ J}$
ダイニン	dyn	$1 \text{ dyn}=10^{-5} \text{ N}$
ボアズ	P	$1 \text{ P}=1 \text{ dyn} \cdot s/cm^2=0.1 \text{ Pa} \cdot s$
ストークス	St	$1 \text{ St}=1 \text{ cm}^2/s=10^{-4} \text{ m/s}$
ガウス	G	$1 \text{ G}=\Delta 10^{-4} \text{ T}$
エルステッド	Oe	$1 \text{ Oe}=\Delta(1000/4\pi) \text{ A/m}$
マクスウェル	Mx	$1 \text{ Mx}=\Delta 10^{-8} \text{ Wb}$
スチール	sb	$1 \text{ sb}=1 \text{ cd}/\text{cm}^2=10^4 \text{ cd/m}^2$
ホル	ph	$1 \text{ ph}=10^4 \text{ lx}$
ガル	Gal	$1 \text{ Gal}=1 \text{ cm/s}^2=10^{-2} \text{ m/s}^2$

表10. 国際単位に属さないその他の単位の例

名称	記号	SI 単位であらわされる数値
キュリ	Ci	$1 Ci=3.7 \times 10^8 \text{ Bq}$
レントゲン	R	$1 R=2.58 \times 10^{-4} \text{ C/kg}$
ラド	rad	$1 rad=1 \text{ Gy}=10^{-2} \text{ Gy}$
レム	rem	$1 rem=1 \text{ cSv}=10^{-2} \text{ Sv}$
X線単位	X unit	$1X \text{ unit}=1.002 \times 10^{-4} \text{ nm}$
ガンマ	γ	$1 \gamma=1 \text{ nT}=10^{-9} \text{ T}$
ジヤンスキー	Jy	$1 Jy=10^{-26} \text{ W} \cdot \text{m}^{-2} \cdot \text{Hz}^{-1}$
フェルミ	fm	$1 \text{ fermi}=1 \text{ fm}=10^{-15} \text{ m}$
メートル系カラット	Torr	$1 \text{ metric carat}=200 \text{ mg}=2 \times 10^{-4} \text{ kg}$
標準大気圧	atm	$1 \text{ Torr}=(101.325/760) \text{ Pa}$
カリ	cal	$1 \text{ atm}=101.325 \text{ Pa}$
ミクロ	μ	$1 \mu=1 \mu \text{m}=10^{-6} \text{ m}$

